Crystallography Open Database for teaching

Saulius Gražulis Andrius Merkys Antanas Vaitkus

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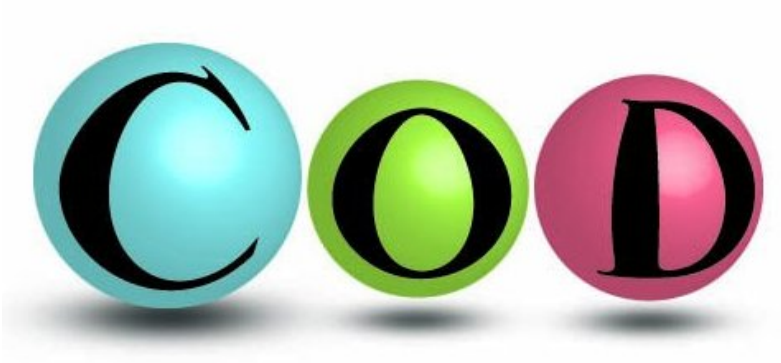
Vilnius University Institute of Biotechnology

This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 689868.

Crystallography Open Database

Largest open-access resource on chemical crystallography



http://www.crystallography.net/

- Total >**380 000** records;
- Grows about 30-50 thous. records/year;

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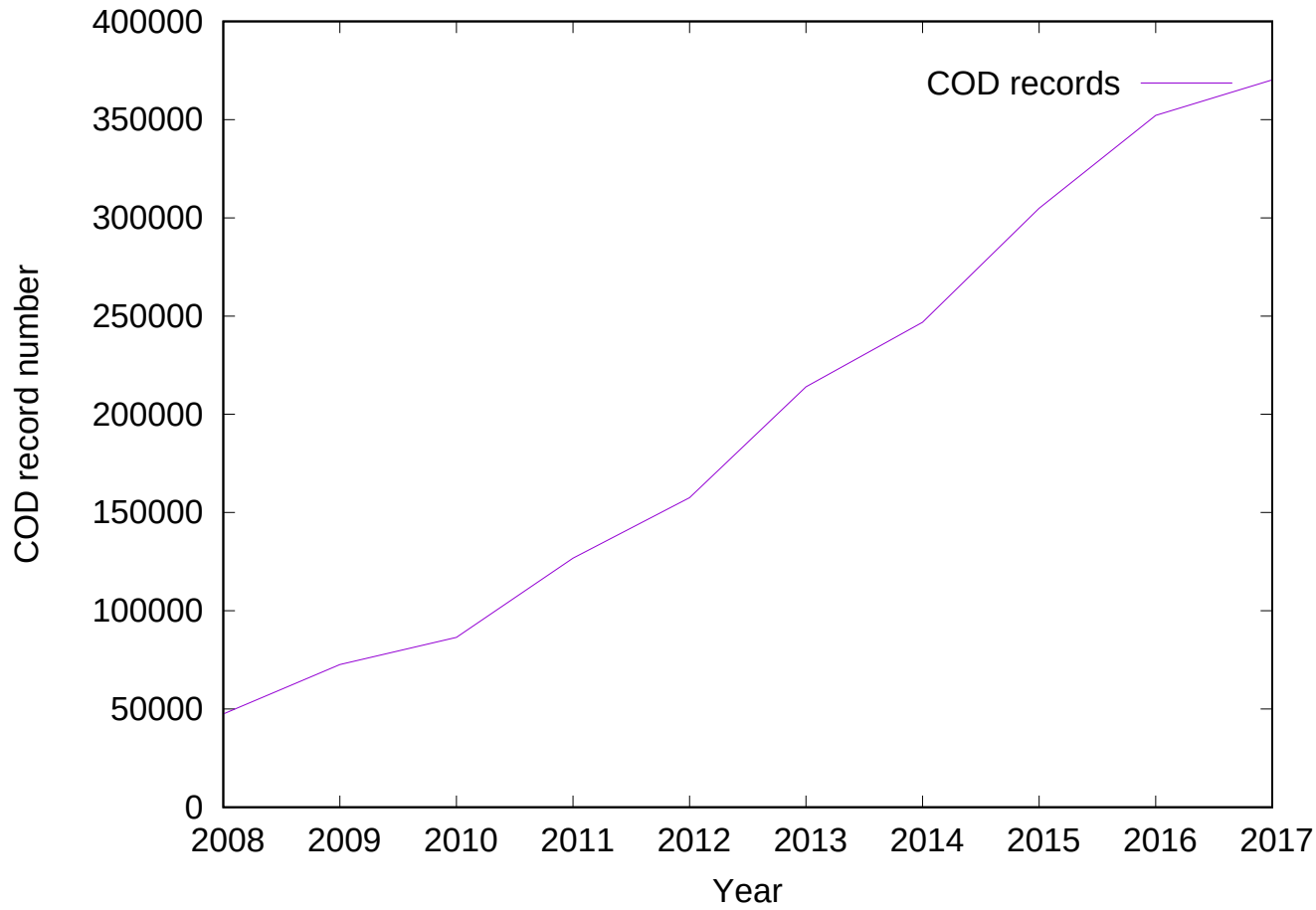
COD persistence

COD is on-line since 2003, growing all the time.



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COD accessibility

COD is a **fully open-access database**. All records are available under public domain designation.

Every crystallographer can contribute data to COD (and many do ;).

Provided access methods are:

- Web search
- URLs constructed from stable identifiers
- RESTful interfaces
- Full data download

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Use of COD for teaching crystallography

We can and may use COD for teaching in following ways:

- as a source of crystallographic information – to illustrate concepts of crystallography;
- as a programmatically accessible resource – to teach data processing and management skills on real-life sized repositories;
- as an goal in itself – students can participate in COD co-development;

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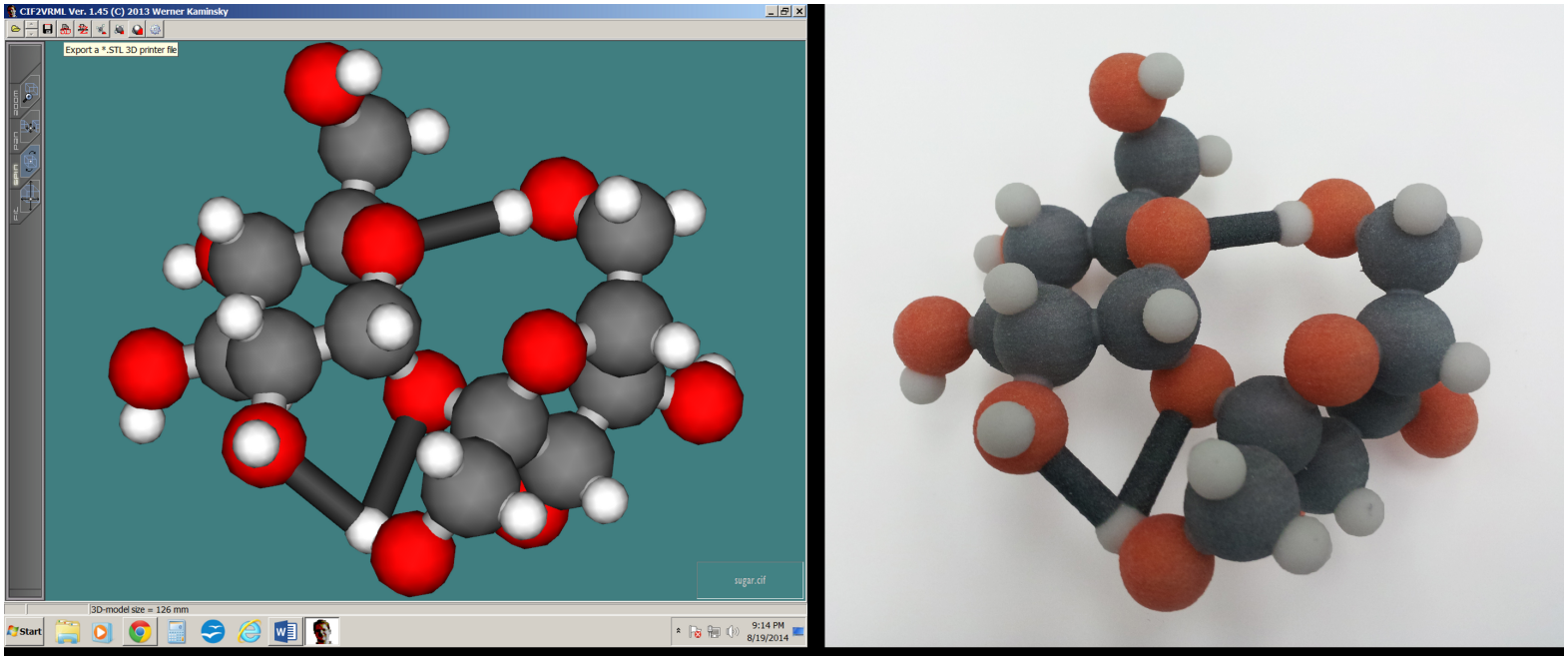
3D printing of models

Use COD to produce 3D Virtual reality descriptions and to eventually make 3D printed models [Kaminsky et al., 2014, Gražulis et al., 2015]:



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Personal story: Andrius Merkys

- Defended his BSc in Bioinformatics (Vilnius University), designed and implemented data deposition interface for the Crystallography Open Database;
- Defended master thesis with honours (Vilnius University), providing the Crystallography Open Database as a source of data for MM model refinement;
- Part of results published together with the group of Garib Murshudov [Long et al., 2017];

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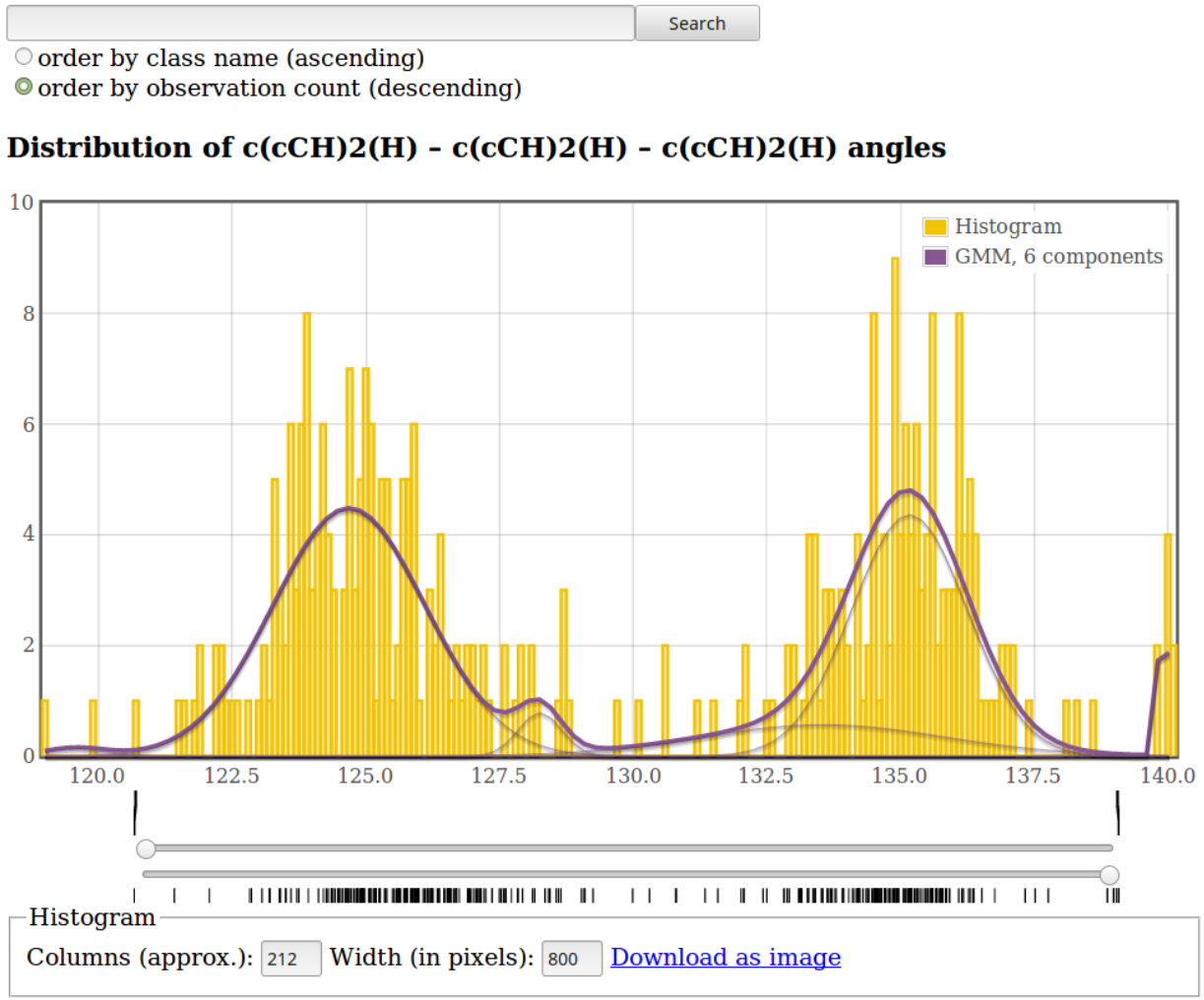
Models in the COD geometry browser

http://www.crystallography.net/geometry/cgi-bin/histogram.pl?class_id=3313-3313-3313



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Personal story: Antanas Vaitkus

- Defended his BSc in Bioinformatics (Vilnius University), on the analysis of interatomic distance distributions in the COD;
- Defended his master thesis (with highest evaluation) on the analysis of metal coordination sphere geometries in COD;
- Works on the PhD thesis; topic: extraction of chemical knowledge from open Web resources and linking them with the COD;

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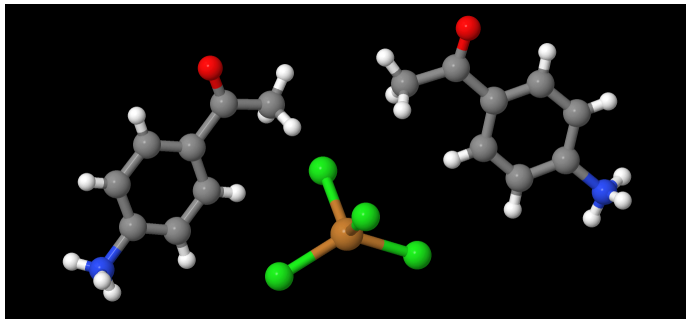
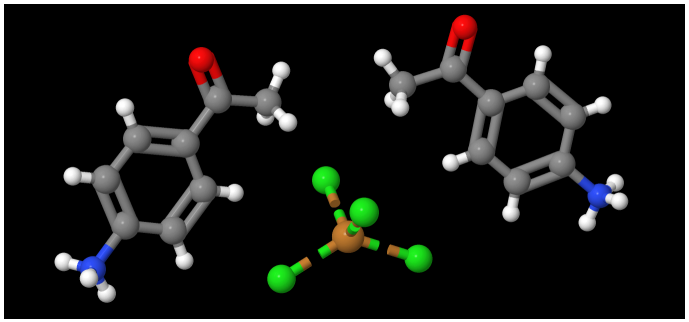
Comprehension of chemical information

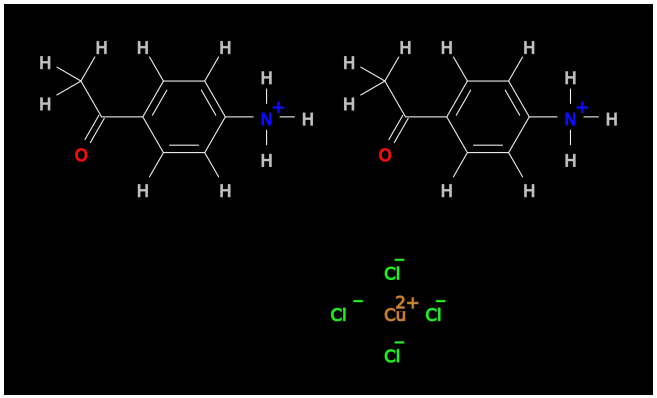
cif_molecule



cif2molecule



Open Babel



[Cu+2]([Cl-])([Cl-])([Cl-])[Cl-].O=C(c1ccc(cc1)[NH3+])C.O=C(c1ccc(cc1)[NH3+])C

Work done with Thomas Sander using his F/LOSS libraries at Actelion

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Personal story: Mélanie Lailler

- Engineer in training at ISTP, in Saint-Etienne (France);
- Visited Vilnius University for 2 months as a part of her internship program;
- In the 2 months, using the open EuropePMC resource, covered software development topics:
  - version control (Subversion);
  - software testing using Make, unite tests, test coverage;
  - software release cycle management;
  - wrote and released a finished program that is planned to be used further for data management int COD and ROD;

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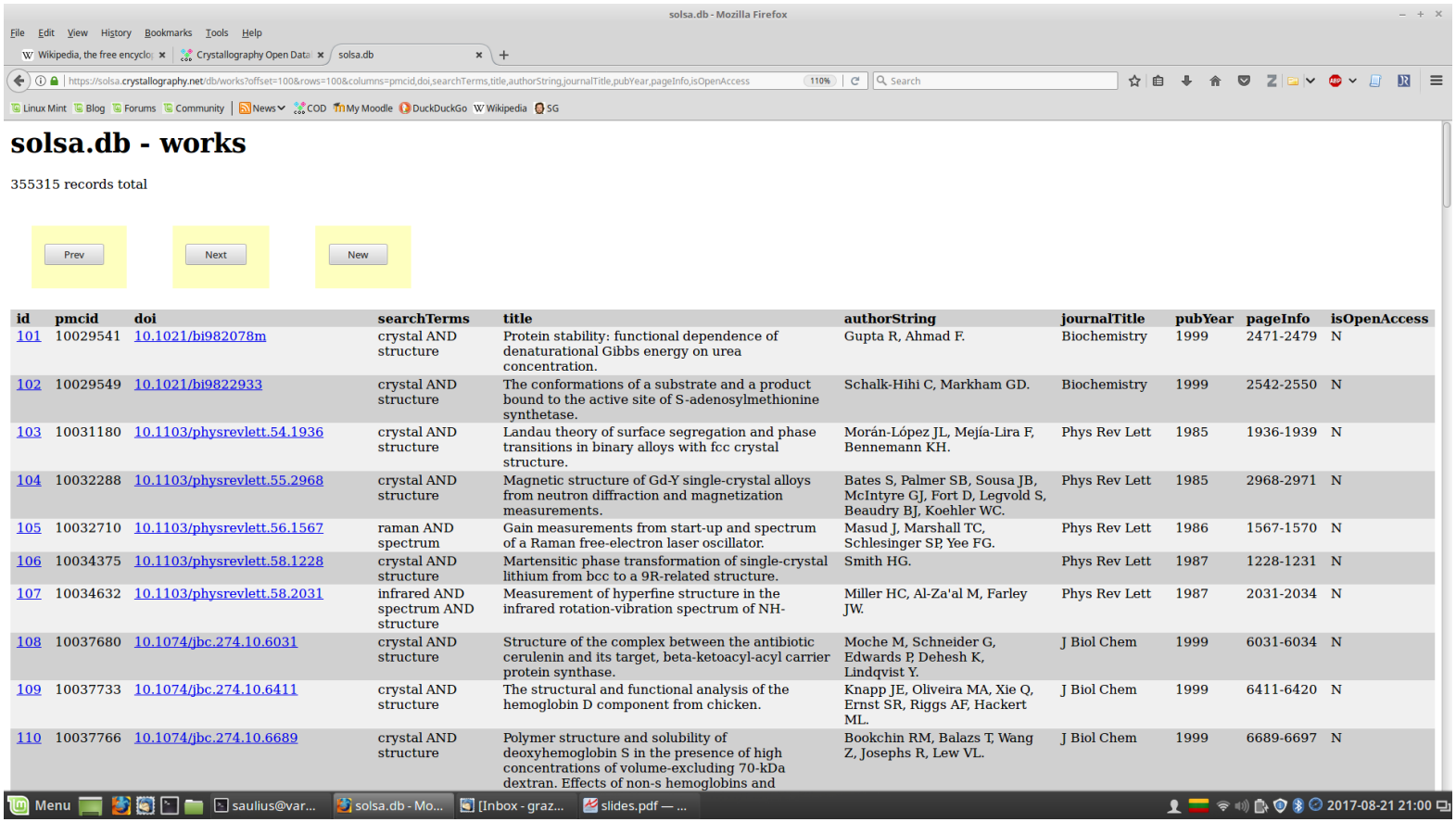
Raman spectra and mineral structures in literature

Automated searches in the open-access EuropePMC resource:



id	pmcid	doi	searchTerms	title	authorString	journalTitle	pubYear	pageInfo	isOpenAccess
101	10029541	10.1021/bi982078m	crystal AND structure	Protein stability: functional dependence of denaturational Gibbs energy on urea concentration.	Gupta R, Ahmad F.	Biochemistry	1999	2471-2479	N
102	10029549	10.1021/bi9822933	crystal AND structure	The conformations of a substrate and a product bound to the active site of S-adenosylmethionine synthetase.	Schalk-Hihi C, Markham GD.	Biochemistry	1999	2542-2550	N
103	10031180	10.1103/physrevlett.54.1936	crystal AND structure	Landau theory of surface segregation and phase transitions in binary alloys with fcc crystal structure.	Morán-López JL, Mejía-Lira F, Bennemann KH.	Phys Rev Lett	1985	1936-1939	N
104	10032288	10.1103/physrevlett.55.2968	crystal AND structure	Magnetic structure of Gd-Y single-crystal alloys from neutron diffraction and magnetization measurements.	Bates S, Palmer SB, Sousa JB, McIntyre GJ, Fort D, Legvold S, Beaudry BJ, Koehler WC.	Phys Rev Lett	1985	2968-2971	N
105	10032710	10.1103/physrevlett.56.1567	raman AND spectrum	Gain measurements from start-up and spectrum of a Raman free-electron laser oscillator.	Masud J, Marshall TC, Schlesinger SP, Yee FG.	Phys Rev Lett	1986	1567-1570	N
106	10034375	10.1103/physrevlett.58.1228	crystal AND structure	Martensitic phase transformation of single-crystal lithium from bcc to a 9R-related structure.	Smith HG.	Phys Rev Lett	1987	1228-1231	N
107	10034632	10.1103/physrevlett.58.2031	infrared AND spectrum AND structure	Measurement of hyperfine structure in the infrared rotation-vibration spectrum of NH-	Miller HC, Al-Za'al M, Farley JW.	Phys Rev Lett	1987	2031-2034	N
108	10037680	10.1074/jbc.274.10.6031	crystal AND structure	Structure of the complex between the antibiotic cerulenin and its target, beta-ketoacyl-acyl carrier protein synthase.	Moche M, Schneider G, Edwards P, Dehesh K, Lindqvist Y.	J Biol Chem	1999	6031-6034	N
109	10037733	10.1074/jbc.274.10.6411	crystal AND structure	The structural and functional analysis of the hemoglobin D component from chicken.	Knapp JE, Oliveira MA, Xie Q, Ernst SR, Riggs AF, Hackert ML.	J Biol Chem	1999	6411-6420	N
110	10037766	10.1074/jbc.274.10.6689	crystal AND structure	Polymer structure and solubility of deoxyhemoglobin S in the presence of high concentrations of volume-excluding 70-kDa dextran. Effects of non-s hemoglobins and	Bookchin RM, Balazs T, Wang Z, Josephs R, Lew VL.	J Biol Chem	1999	6689-6697	N

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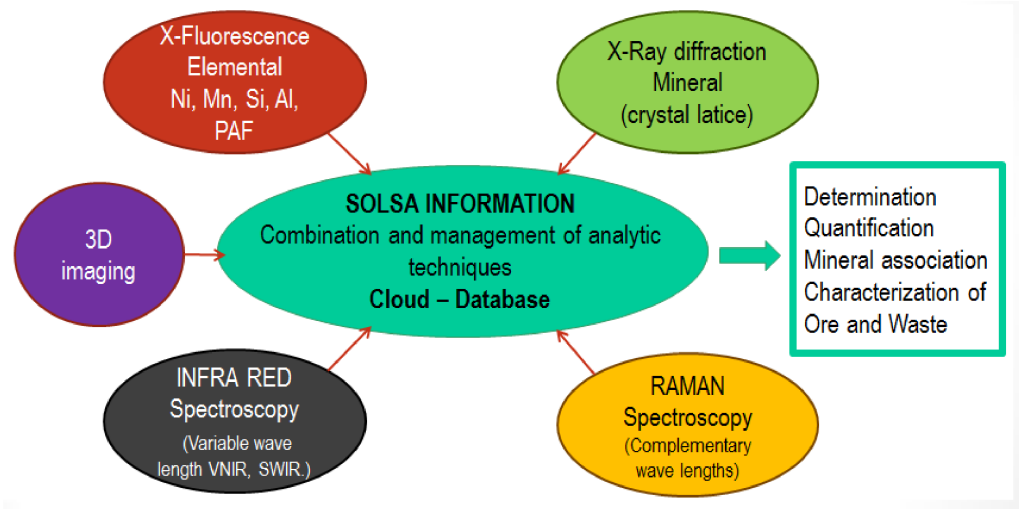
SOLSA project and COD



COD will be used in SOLSA for:

- mineral identification;
- subsequent data dissemination.

SOLSA data flow diagram courtesy Monique Le Guen, ERAMET.

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Contributions of students

- A.V.: design of the CIF dictionaries for Raman, IR, Hyperspectral image databases;
- A.M.: launching and curation of the ROD, HOD and spectral databases;
- M.L.: performed a literature search for potential publications with Raman spectra and crystal structures useful for mineral identification;

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Peter Murray-Rust
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Thank you!

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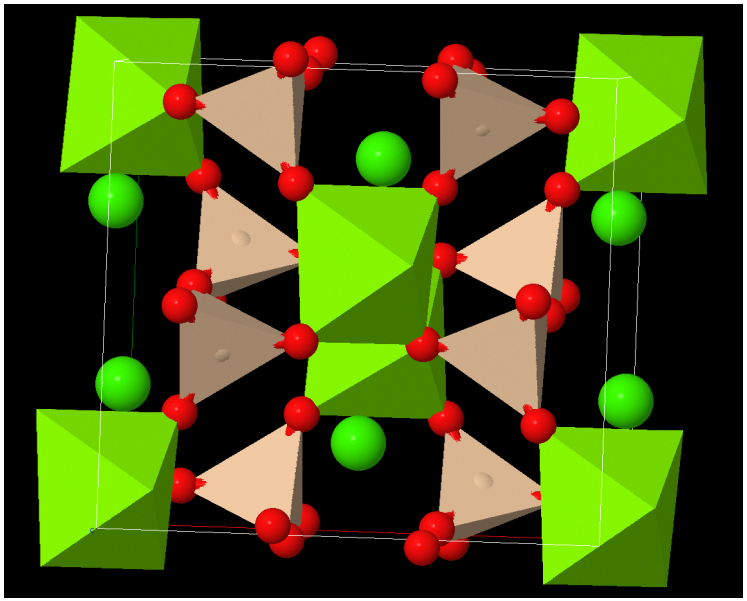

http://www.crystallography.net/1000007.html

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Kaminsky, W., Snyder, T., Stone-Sundberg, J., and Moeck, P. (2014).
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